



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:19 am GMT

PDB ID : 4DEJ
Title : Crystal structure of glutathione transferase-like protein IL0419 (Target EFI-501089) from *Idiomarina loihiensis* L2TR
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Zencheck, W.D.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Imker, H.J.; Armstrong, R.N.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2012-01-20
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

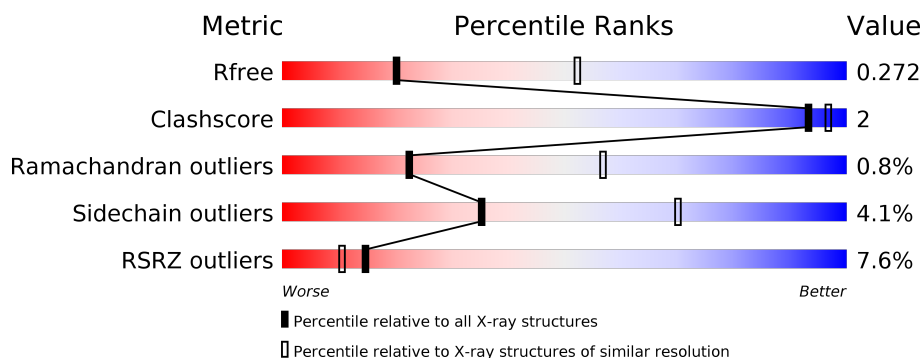
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	231	<div> <div></div> <div> <div>81%</div> <div>5%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	231	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	D	231	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>•</div> <div>•</div> <div>12%</div> </div> </div>
1	E	231	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>•</div> <div>13%</div> </div> </div>
1	F	231	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>6%</div> <div>15%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19591 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutathione S-transferase related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1639	1051	268	312	8			
1	B	201	Total	C	N	O	S	0	0	0
			1634	1048	267	311	8			
1	C	201	Total	C	N	O	S	0	0	0
			1634	1048	267	311	8			
1	D	203	Total	C	N	O	S	0	0	0
			1653	1058	273	314	8			
1	E	200	Total	C	N	O	S	0	0	0
			1625	1042	265	310	8			
1	F	197	Total	C	N	O	S	0	0	0
			1601	1030	258	305	8			
1	G	201	Total	C	N	O	S	0	0	0
			1625	1044	263	310	8			
1	H	201	Total	C	N	O	S	0	0	0
			1636	1048	269	311	8			
1	I	200	Total	C	N	O	S	0	0	0
			1629	1045	266	310	8			
1	J	202	Total	C	N	O	S	0	0	0
			1643	1053	268	314	8			
1	K	201	Total	C	N	O	S	0	0	0
			1640	1051	270	311	8			
1	L	200	Total	C	N	O	S	0	0	0
			1618	1038	263	309	8			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
A	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
A	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
A	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
A	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
A	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
A	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
A	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
A	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
A	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
A	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
A	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
A	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
A	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
A	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
A	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
A	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
B	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
B	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
B	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
B	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
B	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
B	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
B	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
B	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
B	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
B	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
B	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
B	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
B	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
B	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
B	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
B	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
B	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
C	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
C	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
C	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
C	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
C	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
C	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
C	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
C	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
C	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
C	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
C	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
C	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
C	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
C	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
C	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
C	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
C	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
C	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
D	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
D	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
D	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
D	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
D	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
D	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
D	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
D	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
D	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
D	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
D	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
D	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
D	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
D	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
D	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
D	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
D	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
E	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
E	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
E	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
E	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
E	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
E	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
E	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
E	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
E	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
E	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
E	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
E	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
E	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
E	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
E	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
E	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
E	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
E	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
F	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
F	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
F	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
F	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
F	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
F	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
F	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
F	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
F	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
F	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
F	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
F	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
F	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
F	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
F	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
F	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
F	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
F	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
G	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
G	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
G	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
G	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
G	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
G	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
G	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
G	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
G	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
G	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
G	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
G	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
G	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
G	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
G	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
G	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
G	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
G	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
H	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
H	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
H	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
H	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
H	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
H	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
H	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
H	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
H	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
H	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
H	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
H	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
H	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
H	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
H	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
H	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
H	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
I	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
I	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
I	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
I	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
I	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
I	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
I	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
I	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
I	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
I	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
I	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
I	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
I	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
I	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
I	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
I	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
I	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
J	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
J	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
J	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
J	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
J	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
J	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
J	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
J	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
J	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
J	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
J	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
J	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
J	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
J	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
J	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
J	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
J	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
J	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
K	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
K	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
K	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
K	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
K	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
K	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
K	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
K	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
K	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
K	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
K	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
K	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
K	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
K	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
K	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
K	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
K	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1
L	-1	MET	-	EXPRESSION TAG	UNP Q5R0K1
L	0	VAL	-	EXPRESSION TAG	UNP Q5R0K1
L	208	ALA	-	EXPRESSION TAG	UNP Q5R0K1
L	209	GLU	-	EXPRESSION TAG	UNP Q5R0K1
L	210	ASN	-	EXPRESSION TAG	UNP Q5R0K1
L	211	LEU	-	EXPRESSION TAG	UNP Q5R0K1
L	212	TYR	-	EXPRESSION TAG	UNP Q5R0K1
L	213	PHE	-	EXPRESSION TAG	UNP Q5R0K1
L	214	GLN	-	EXPRESSION TAG	UNP Q5R0K1
L	215	SER	-	EXPRESSION TAG	UNP Q5R0K1
L	216	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	217	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	218	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	219	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	220	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	221	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	222	TRP	-	EXPRESSION TAG	UNP Q5R0K1
L	223	SER	-	EXPRESSION TAG	UNP Q5R0K1
L	224	HIS	-	EXPRESSION TAG	UNP Q5R0K1
L	225	PRO	-	EXPRESSION TAG	UNP Q5R0K1
L	226	GLN	-	EXPRESSION TAG	UNP Q5R0K1
L	227	PHE	-	EXPRESSION TAG	UNP Q5R0K1
L	228	GLU	-	EXPRESSION TAG	UNP Q5R0K1
L	229	LYS	-	EXPRESSION TAG	UNP Q5R0K1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	3	Total O 3 3	0	0
2	C	1	Total O 1 1	0	0
2	E	1	Total O 1 1	0	0

Continued on next page...

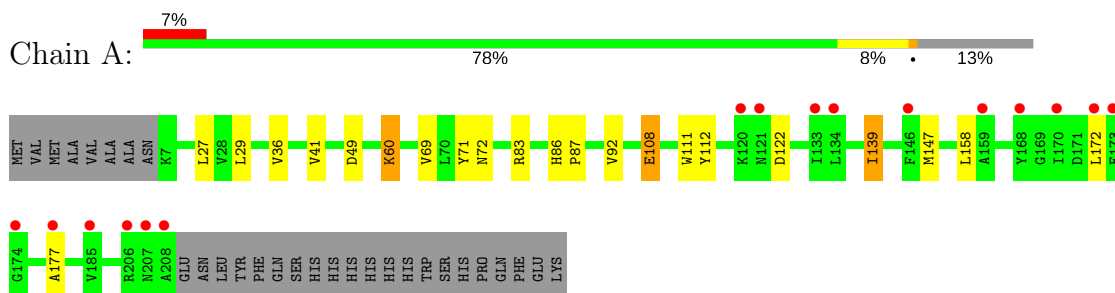
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	O 1	0	0
2	I	2	Total 2	O 2	0	0
2	J	1	Total 1	O 1	0	0
2	L	1	Total 1	O 1	0	0

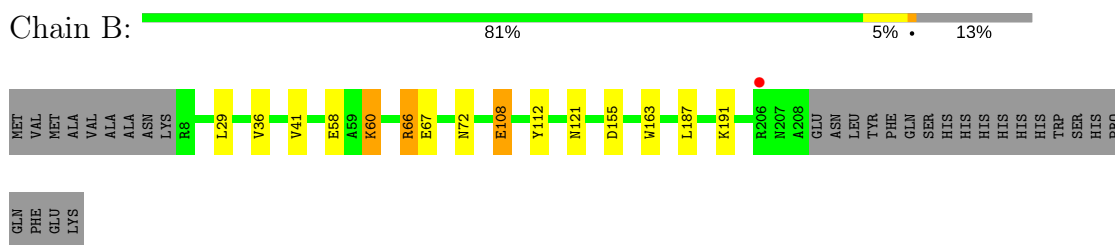
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

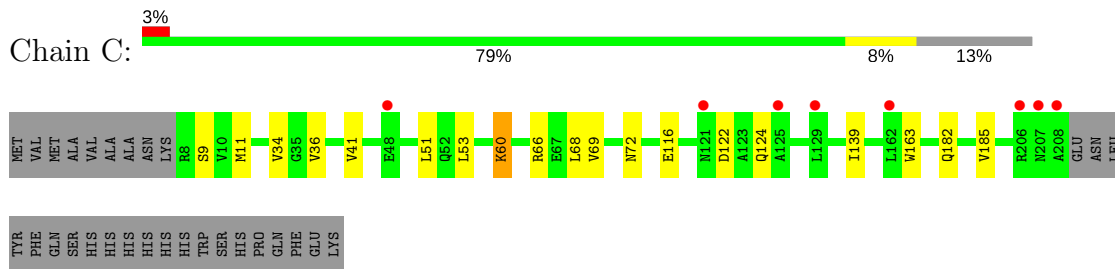
- Molecule 1: Glutathione S-transferase related protein



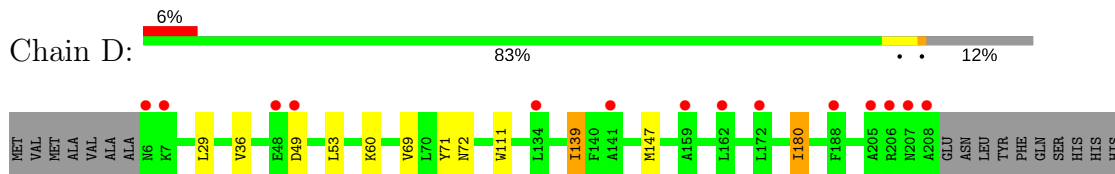
- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein




- Molecule 1: Glutathione S-transferase related protein



HIS
HIS
HIS
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS


- Molecule 1: Glutathione S-transferase related protein

Chain E: 

MET VAL MET MET VAL ALA VAL ALA ALA ASN LYS TRP SER HIS PRO GLN PHE GLU LYS

TYR PHE GLN SER SER HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS


- Molecule 1: Glutathione S-transferase related protein

Chain F: 

MET VAL MET MET VAL ALA ALA ALA ASN LYS TRP SER HIS PRO GLN PHE GLU LYS

VAL MET MET VAL ALA ALA ALA ASN LYS TRP SER HIS PRO GLN PHE GLU LYS


- Molecule 1: Glutathione S-transferase related protein

Chain G: 

MET VAL MET MET VAL ALA ALA ALA ASN LYS TRP SER HIS PRO GLN PHE GLU LYS

GLU ASN LYS TRP SER HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS


- Molecule 1: Glutathione S-transferase related protein

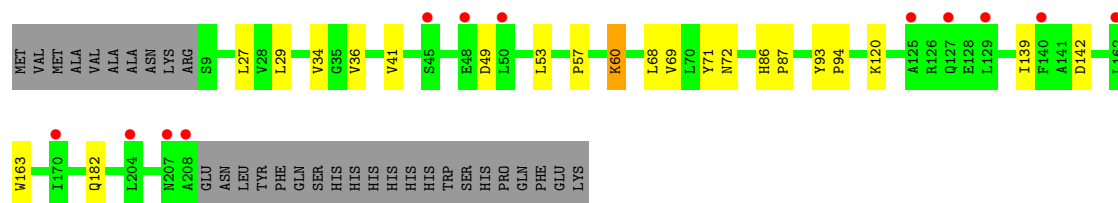
Chain H: 

MET VAL MET MET VAL ALA ALA ALA ASN LYS TRP SER HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS

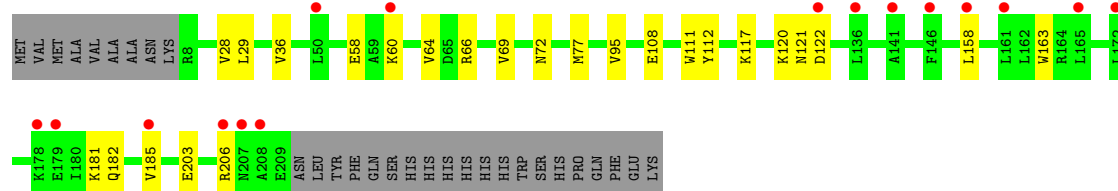
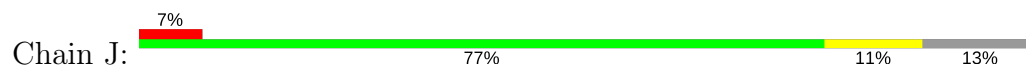
VAL MET MET VAL ALA ALA ALA ASN LYS TRP SER HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 1: Glutathione S-transferase related protein

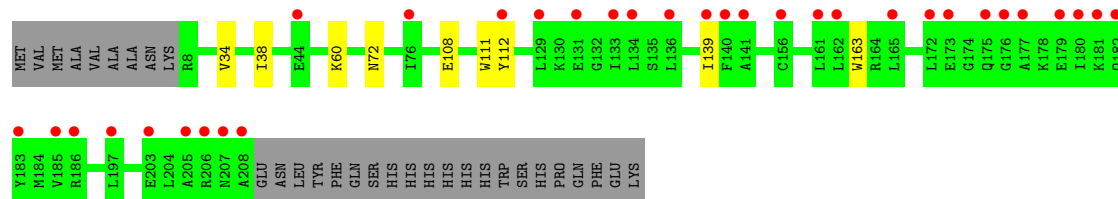
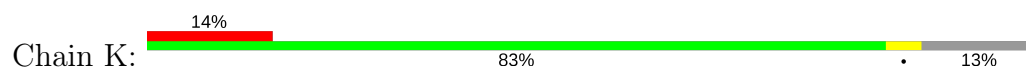
Chain I: 



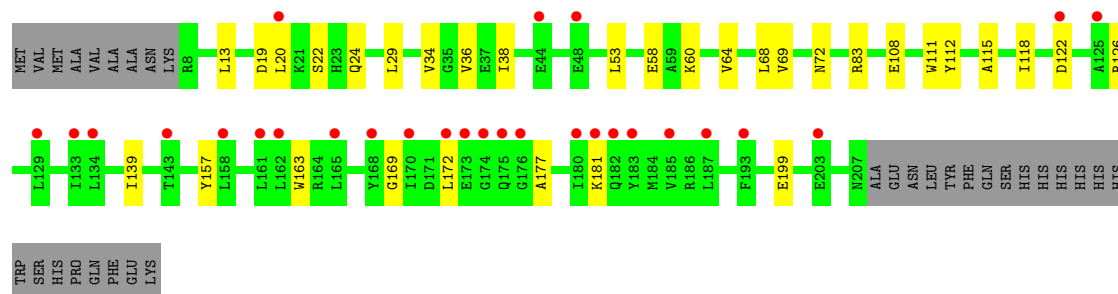
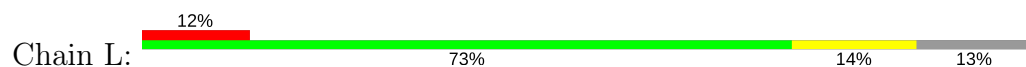
- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.36Å 156.99Å 244.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 48.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.90) 99.1 (48.10-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.275 0.210 , 0.272	Depositor DCC
R_{free} test set	2359 reflections (3.10%)	DCC
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19591	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	1/1675 (0.1%)	0.62	0/2271
1	B	0.43	1/1670 (0.1%)	0.64	0/2264
1	C	0.42	1/1670 (0.1%)	0.62	0/2264
1	D	0.43	1/1689 (0.1%)	0.61	0/2289
1	E	0.43	0/1661	0.63	0/2253
1	F	0.43	1/1637 (0.1%)	0.60	0/2220
1	G	0.43	0/1661	0.62	0/2253
1	H	0.44	2/1672 (0.1%)	0.61	0/2267
1	I	0.42	1/1665 (0.1%)	0.61	0/2257
1	J	0.43	2/1679 (0.1%)	0.59	0/2276
1	K	0.43	2/1676 (0.1%)	0.60	0/2271
1	L	0.43	2/1654 (0.1%)	0.59	0/2245
All	All	0.43	14/20009 (0.1%)	0.61	0/27130

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	111	TRP	CD2-CE2	5.29	1.47	1.41
1	A	111	TRP	CD2-CE2	5.27	1.47	1.41
1	F	111	TRP	CD2-CE2	5.26	1.47	1.41
1	D	111	TRP	CD2-CE2	5.19	1.47	1.41
1	H	163	TRP	CD2-CE2	5.18	1.47	1.41
1	L	163	TRP	CD2-CE2	5.17	1.47	1.41
1	K	111	TRP	CD2-CE2	5.11	1.47	1.41
1	C	163	TRP	CD2-CE2	5.09	1.47	1.41
1	H	111	TRP	CD2-CE2	5.08	1.47	1.41
1	B	163	TRP	CD2-CE2	5.07	1.47	1.41
1	K	163	TRP	CD2-CE2	5.07	1.47	1.41
1	L	111	TRP	CD2-CE2	5.07	1.47	1.41
1	I	163	TRP	CD2-CE2	5.06	1.47	1.41
1	J	163	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1639	0	1627	6	0
1	B	1634	0	1625	5	0
1	C	1634	0	1625	3	0
1	D	1653	0	1644	4	0
1	E	1625	0	1612	7	0
1	F	1601	0	1593	4	0
1	G	1625	0	1610	5	0
1	H	1636	0	1625	6	0
1	I	1629	0	1623	7	0
1	J	1643	0	1631	10	0
1	K	1640	0	1636	2	0
1	L	1618	0	1594	11	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
2	L	1	0	0	0	0
All	All	19591	0	19445	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:ASN:O	1:J:121:ASN:ND2	2.30	0.64
1:I:29:LEU:HD13	1:I:36:VAL:HG11	1.85	0.57
1:E:29:LEU:HD13	1:E:36:VAL:HG11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:LYS:O	1:J:121:ASN:HB3	2.06	0.56
1:L:29:LEU:HD13	1:L:36:VAL:HG11	1.88	0.56
1:A:172:LEU:HB2	1:A:177:ALA:HB1	1.88	0.55
1:B:29:LEU:HD13	1:B:36:VAL:HG11	1.88	0.55
1:A:108:GLU:HA	1:A:112:TYR:HB2	1.89	0.55
1:A:41:VAL:HG23	1:A:60:LYS:HE3	1.89	0.54
1:C:53:LEU:HB3	1:C:69:VAL:HG21	1.89	0.53
1:J:117:LYS:HB3	1:J:122:ASP:OD2	2.08	0.53
1:D:139:ILE:HD13	1:D:147:MET:HG3	1.91	0.53
1:A:29:LEU:HD13	1:A:36:VAL:HG11	1.89	0.52
1:J:29:LEU:HD13	1:J:36:VAL:HG11	1.91	0.52
1:L:53:LEU:HB3	1:L:69:VAL:HG21	1.92	0.52
1:E:42:THR:HG23	1:E:45:SER:H	1.76	0.51
1:D:29:LEU:HD13	1:D:36:VAL:HG11	1.94	0.50
1:I:41:VAL:HG23	1:I:60:LYS:HE3	1.93	0.50
1:F:29:LEU:HD13	1:F:36:VAL:HG11	1.93	0.50
1:D:53:LEU:HB3	1:D:69:VAL:HG21	1.94	0.50
1:G:108:GLU:HA	1:G:112:TYR:HB2	1.94	0.49
1:I:53:LEU:HB3	1:I:69:VAL:HG21	1.93	0.49
1:F:53:LEU:HB3	1:F:69:VAL:HG21	1.93	0.49
1:L:24:GLN:HE21	1:L:157:TYR:HA	1.78	0.48
1:G:53:LEU:HB3	1:G:69:VAL:HG21	1.95	0.48
1:H:24:GLN:HE21	1:H:157:TYR:HA	1.79	0.47
1:J:108:GLU:HA	1:J:112:TYR:HB2	1.96	0.47
1:E:34:VAL:HG12	1:L:34:VAL:HG13	1.97	0.47
1:A:139:ILE:HD13	1:A:147:MET:HG3	1.96	0.46
1:C:11:MET:HB2	1:C:36:VAL:HG12	1.97	0.46
1:L:108:GLU:HA	1:L:112:TYR:HB2	1.97	0.46
1:E:72:ASN:HB3	1:E:75:ILE:HD12	1.98	0.45
1:L:115:ALA:HA	1:L:118:ILE:HD12	1.98	0.45
1:C:41:VAL:HG23	1:C:60:LYS:HE3	1.98	0.45
1:H:29:LEU:HD13	1:H:36:VAL:HG11	1.98	0.45
1:L:126:ARG:HE	1:L:169:GLY:HA3	1.82	0.45
1:B:41:VAL:HG23	1:B:60:LYS:HE3	1.98	0.45
1:I:34:VAL:HG12	1:K:34:VAL:HG13	1.99	0.45
1:B:155:ASP:HB3	1:B:187:LEU:HD11	2.00	0.44
1:A:86:HIS:HA	1:A:87:PRO:HA	1.91	0.44
1:H:172:LEU:HB3	1:H:177:ALA:HB1	1.98	0.44
1:J:203:GLU:HG3	1:J:206:ARG:HH11	1.82	0.44
1:L:172:LEU:HD22	1:L:177:ALA:HB1	2.00	0.44
1:F:41:VAL:HG23	1:F:60:LYS:HE3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:TYR:HA	1:I:94:PRO:HD3	1.87	0.43
1:E:41:VAL:HG23	1:E:60:LYS:HE3	1.99	0.43
1:J:28:VAL:HG21	1:J:77:MET:HG2	2.01	0.42
1:L:64:VAL:HG22	1:L:69:VAL:HG23	2.01	0.42
1:E:24:GLN:HE21	1:E:157:TYR:HA	1.84	0.42
1:I:68:LEU:HD22	1:J:95:VAL:HG13	2.01	0.42
1:K:108:GLU:HA	1:K:112:TYR:HB2	2.02	0.42
1:G:162:LEU:HA	1:G:165:LEU:HD13	2.01	0.42
1:L:13:LEU:HD23	1:L:38:ILE:HG12	2.01	0.42
1:H:53:LEU:HD13	1:H:64:VAL:HG21	2.01	0.42
1:B:66:ARG:HB2	1:B:67:GLU:H	1.73	0.42
1:G:137:ALA:HA	1:G:140:PHE:HD2	1.85	0.42
1:J:120:LYS:O	1:J:121:ASN:CB	2.65	0.42
1:G:74:GLN:HE21	1:G:78:GLU:HG3	1.84	0.41
1:H:93:TYR:HA	1:H:94:PRO:HD3	1.92	0.41
1:J:64:VAL:HG22	1:J:69:VAL:HG23	2.01	0.41
1:I:86:HIS:HA	1:I:87:PRO:HA	1.94	0.41
1:F:24:GLN:HE21	1:F:157:TYR:HA	1.85	0.41
1:H:108:GLU:HA	1:H:112:TYR:HB2	2.02	0.41
1:L:19:ASP:HB3	1:L:22:SER:HB2	2.03	0.41
1:D:180:ILE:HG12	1:D:180:ILE:H	1.69	0.41
1:E:53:LEU:HB3	1:E:69:VAL:HG21	2.03	0.40
1:B:108:GLU:HA	1:B:112:TYR:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	200/231 (87%)	191 (96%)	8 (4%)	1 (0%)	32 68
1	B	199/231 (86%)	195 (98%)	2 (1%)	2 (1%)	18 51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	199/231 (86%)	189 (95%)	8 (4%)	2 (1%)	18	51
1	D	201/231 (87%)	195 (97%)	5 (2%)	1 (0%)	32	68
1	E	198/231 (86%)	194 (98%)	2 (1%)	2 (1%)	18	51
1	F	195/231 (84%)	189 (97%)	5 (3%)	1 (0%)	32	68
1	G	199/231 (86%)	192 (96%)	5 (2%)	2 (1%)	18	51
1	H	199/231 (86%)	193 (97%)	3 (2%)	3 (2%)	12	39
1	I	198/231 (86%)	191 (96%)	5 (2%)	2 (1%)	18	51
1	J	200/231 (87%)	194 (97%)	4 (2%)	2 (1%)	18	51
1	K	199/231 (86%)	188 (94%)	10 (5%)	1 (0%)	32	68
1	L	198/231 (86%)	190 (96%)	7 (4%)	1 (0%)	32	68
All	All	2385/2772 (86%)	2301 (96%)	64 (3%)	20 (1%)	22	57

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	B	72	ASN
1	E	66	ARG
1	F	72	ASN
1	G	66	ARG
1	H	66	ARG
1	H	120	LYS
1	J	66	ARG
1	K	72	ASN
1	L	72	ASN
1	B	66	ARG
1	D	72	ASN
1	E	72	ASN
1	G	72	ASN
1	H	72	ASN
1	I	72	ASN
1	J	72	ASN
1	C	66	ARG
1	C	72	ASN
1	I	120	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/206 (86%)	167 (94%)	11 (6%)	21	52
1	B	178/206 (86%)	173 (97%)	5 (3%)	49	82
1	C	178/206 (86%)	167 (94%)	11 (6%)	21	52
1	D	180/206 (87%)	175 (97%)	5 (3%)	49	82
1	E	177/206 (86%)	172 (97%)	5 (3%)	49	82
1	F	175/206 (85%)	170 (97%)	5 (3%)	48	81
1	G	176/206 (85%)	166 (94%)	10 (6%)	24	56
1	H	178/206 (86%)	168 (94%)	10 (6%)	25	57
1	I	178/206 (86%)	170 (96%)	8 (4%)	32	66
1	J	179/206 (87%)	173 (97%)	6 (3%)	42	76
1	K	179/206 (87%)	176 (98%)	3 (2%)	66	89
1	L	175/206 (85%)	166 (95%)	9 (5%)	28	62
All	All	2131/2472 (86%)	2043 (96%)	88 (4%)	35	70

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	49	ASP
1	A	60	LYS
1	A	69	VAL
1	A	71	TYR
1	A	83	ARG
1	A	92	VAL
1	A	108	GLU
1	A	122	ASP
1	A	139	ILE
1	A	158	LEU
1	B	58	GLU
1	B	60	LYS
1	B	108	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	121	ASN
1	B	191	LYS
1	C	9	SER
1	C	34	VAL
1	C	51	LEU
1	C	60	LYS
1	C	68	LEU
1	C	116	GLU
1	C	122	ASP
1	C	124	GLN
1	C	139	ILE
1	C	182	GLN
1	C	185	VAL
1	D	49	ASP
1	D	60	LYS
1	D	71	TYR
1	D	139	ILE
1	D	180	ILE
1	E	27	LEU
1	E	42	THR
1	E	49	ASP
1	E	60	LYS
1	E	83	ARG
1	F	27	LEU
1	F	60	LYS
1	F	121	ASN
1	F	139	ILE
1	F	158	LEU
1	G	36	VAL
1	G	60	LYS
1	G	68	LEU
1	G	71	TYR
1	G	83	ARG
1	G	108	GLU
1	G	139	ILE
1	G	172	LEU
1	G	175	GLN
1	G	195	ASP
1	H	8	ARG
1	H	27	LEU
1	H	49	ASP
1	H	60	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	71	TYR
1	H	83	ARG
1	H	92	VAL
1	H	122	ASP
1	H	139	ILE
1	H	191	LYS
1	I	27	LEU
1	I	49	ASP
1	I	57	PRO
1	I	60	LYS
1	I	71	TYR
1	I	139	ILE
1	I	142	ASP
1	I	182	GLN
1	J	58	GLU
1	J	60	LYS
1	J	158	LEU
1	J	181	LYS
1	J	182	GLN
1	J	185	VAL
1	K	38	ILE
1	K	60	LYS
1	K	139	ILE
1	L	20	LEU
1	L	58	GLU
1	L	60	LYS
1	L	68	LEU
1	L	83	ARG
1	L	122	ASP
1	L	139	ILE
1	L	181	LYS
1	L	199	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	B	24	GLN
1	B	127	GLN
1	E	24	GLN
1	F	24	GLN
1	F	182	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	182	GLN
1	H	24	GLN
1	H	119	GLN
1	I	24	GLN
1	I	119	GLN
1	J	52	GLN
1	J	121	ASN
1	J	182	GLN
1	K	182	GLN
1	L	24	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	202/231 (87%)	0.60	16 (7%) 13 10	57, 94, 148, 176	0
1	B	201/231 (87%)	0.31	1 (0%) 90 90	47, 77, 123, 184	0
1	C	201/231 (87%)	0.40	8 (3%) 39 34	56, 93, 142, 173	0
1	D	203/231 (87%)	0.56	14 (6%) 18 13	63, 95, 144, 173	0
1	E	200/231 (86%)	0.50	9 (4%) 34 29	56, 84, 140, 184	0
1	F	197/231 (85%)	0.63	16 (8%) 13 9	59, 103, 151, 169	0
1	G	201/231 (87%)	0.69	14 (6%) 17 12	55, 100, 149, 180	0
1	H	201/231 (87%)	0.52	15 (7%) 15 11	69, 105, 150, 169	0
1	I	200/231 (86%)	0.47	12 (6%) 23 17	67, 101, 147, 188	0
1	J	202/231 (87%)	0.54	16 (7%) 13 10	68, 104, 149, 187	0
1	K	201/231 (87%)	0.96	33 (16%) 2 1	76, 124, 163, 180	0
1	L	200/231 (86%)	0.85	28 (14%) 3 2	76, 126, 165, 182	0
All	All	2409/2772 (86%)	0.59	182 (7%) 15 10	47, 100, 155, 188	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	208	ALA	7.7
1	G	207	ASN	6.9
1	D	6	ASN	6.2
1	L	183	TYR	6.2
1	K	185	VAL	6.0
1	L	168	TYR	5.9
1	A	121	ASN	5.8
1	K	172	LEU	5.6
1	G	173	GLU	5.2
1	L	162	LEU	5.1
1	A	173	GLU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	207	ASN	4.7
1	D	206	ARG	4.6
1	C	121	ASN	4.6
1	F	176	GLY	4.5
1	E	48	GLU	4.5
1	L	175	GLN	4.5
1	L	125	ALA	4.3
1	F	180	ILE	4.3
1	L	176	GLY	4.2
1	J	207	ASN	4.1
1	L	158	LEU	4.1
1	L	165	LEU	4.1
1	L	129	LEU	4.1
1	L	172	LEU	4.1
1	J	208	ALA	4.1
1	H	134	LEU	4.0
1	G	208	ALA	4.0
1	J	136	LEU	3.9
1	G	174	GLY	3.9
1	G	140	PHE	3.8
1	I	45	SER	3.8
1	G	141	ALA	3.8
1	K	156	CYS	3.7
1	D	205	ALA	3.6
1	D	208	ALA	3.6
1	D	48	GLU	3.6
1	A	207	ASN	3.6
1	L	161	LEU	3.5
1	E	123	ALA	3.5
1	K	181	LYS	3.4
1	L	133	ILE	3.4
1	K	206	ARG	3.4
1	L	44	GLU	3.4
1	I	207	ASN	3.4
1	K	131	GLU	3.3
1	K	162	LEU	3.3
1	A	174	GLY	3.3
1	K	183	TYR	3.3
1	L	187	LEU	3.2
1	J	185	VAL	3.2
1	E	50	LEU	3.2
1	L	173	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	206	ARG	3.2
1	I	208	ALA	3.2
1	G	204	LEU	3.2
1	K	180	ILE	3.2
1	I	127	GLN	3.2
1	K	44	GLU	3.2
1	D	172	LEU	3.2
1	A	134	LEU	3.1
1	G	206	ARG	3.1
1	K	175	GLN	3.1
1	D	162	LEU	3.1
1	A	172	LEU	3.0
1	L	122	ASP	3.0
1	F	44	GLU	3.0
1	K	129	LEU	3.0
1	E	45	SER	3.0
1	F	177	ALA	3.0
1	A	133	ILE	3.0
1	D	49	ASP	2.9
1	F	161	LEU	2.9
1	F	174	GLY	2.9
1	L	181	LYS	2.9
1	H	121	ASN	2.9
1	A	208	ALA	2.9
1	A	146	PHE	2.9
1	L	48	GLU	2.8
1	K	140	PHE	2.8
1	G	44	GLU	2.8
1	K	203	GLU	2.8
1	F	185	VAL	2.8
1	L	185	VAL	2.8
1	F	199	GLU	2.8
1	A	168	TYR	2.8
1	D	207	ASN	2.7
1	K	133	ILE	2.7
1	A	170	ILE	2.7
1	I	204	LEU	2.7
1	K	186	ARG	2.7
1	J	172	LEU	2.7
1	K	134	LEU	2.7
1	E	67	GLU	2.7
1	F	45	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	170	ILE	2.7
1	L	134	LEU	2.7
1	L	174	GLY	2.7
1	F	172	LEU	2.6
1	K	136	LEU	2.6
1	K	141	ALA	2.6
1	K	177	ALA	2.6
1	J	178	LYS	2.6
1	H	133	ILE	2.6
1	K	182	GLN	2.6
1	G	159	ALA	2.6
1	J	179	GLU	2.6
1	C	125	ALA	2.6
1	D	159	ALA	2.6
1	G	178	LYS	2.6
1	D	141	ALA	2.5
1	F	134	LEU	2.5
1	B	206	ARG	2.5
1	K	173	GLU	2.5
1	L	180	ILE	2.5
1	D	134	LEU	2.5
1	K	179	GLU	2.5
1	L	143	THR	2.5
1	C	48	GLU	2.4
1	I	50	LEU	2.4
1	I	129	LEU	2.4
1	K	139	ILE	2.4
1	J	206	ARG	2.4
1	K	205	ALA	2.4
1	K	76	ILE	2.4
1	L	193	PHE	2.3
1	K	197	LEU	2.3
1	G	176	GLY	2.3
1	J	122	ASP	2.3
1	J	141	ALA	2.3
1	E	20	LEU	2.3
1	C	208	ALA	2.3
1	L	203	GLU	2.3
1	C	129	LEU	2.3
1	I	48	GLU	2.3
1	H	162	LEU	2.3
1	H	53	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	175	GLN	2.3
1	A	177	ALA	2.3
1	J	158	LEU	2.3
1	K	176	GLY	2.3
1	C	162	LEU	2.3
1	F	136	LEU	2.3
1	A	120	LYS	2.3
1	H	165	LEU	2.2
1	H	181	LYS	2.2
1	D	188	PHE	2.2
1	A	206	ARG	2.2
1	I	125	ALA	2.2
1	K	161	LEU	2.2
1	L	170	ILE	2.2
1	H	185	VAL	2.2
1	F	121	ASN	2.2
1	F	173	GLU	2.2
1	I	162	LEU	2.2
1	L	20	LEU	2.2
1	J	146	PHE	2.2
1	D	7	LYS	2.2
1	H	158	LEU	2.2
1	J	161	LEU	2.2
1	A	185	VAL	2.2
1	H	208	ALA	2.2
1	E	51	LEU	2.1
1	A	159	ALA	2.1
1	G	180	ILE	2.1
1	L	182	GLN	2.1
1	F	178	LYS	2.1
1	E	170	ILE	2.1
1	H	130	LYS	2.1
1	K	207	ASN	2.1
1	J	165	LEU	2.1
1	H	124	GLN	2.1
1	K	112	TYR	2.1
1	J	50	LEU	2.0
1	H	177	ALA	2.0
1	H	44	GLU	2.0
1	K	165	LEU	2.0
1	H	159	ALA	2.0
1	I	140	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	44	GLU	2.0
1	F	154	VAL	2.0
1	J	60	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.